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Field-scale investigation of microbially induced calcite precipitation using a numerical model

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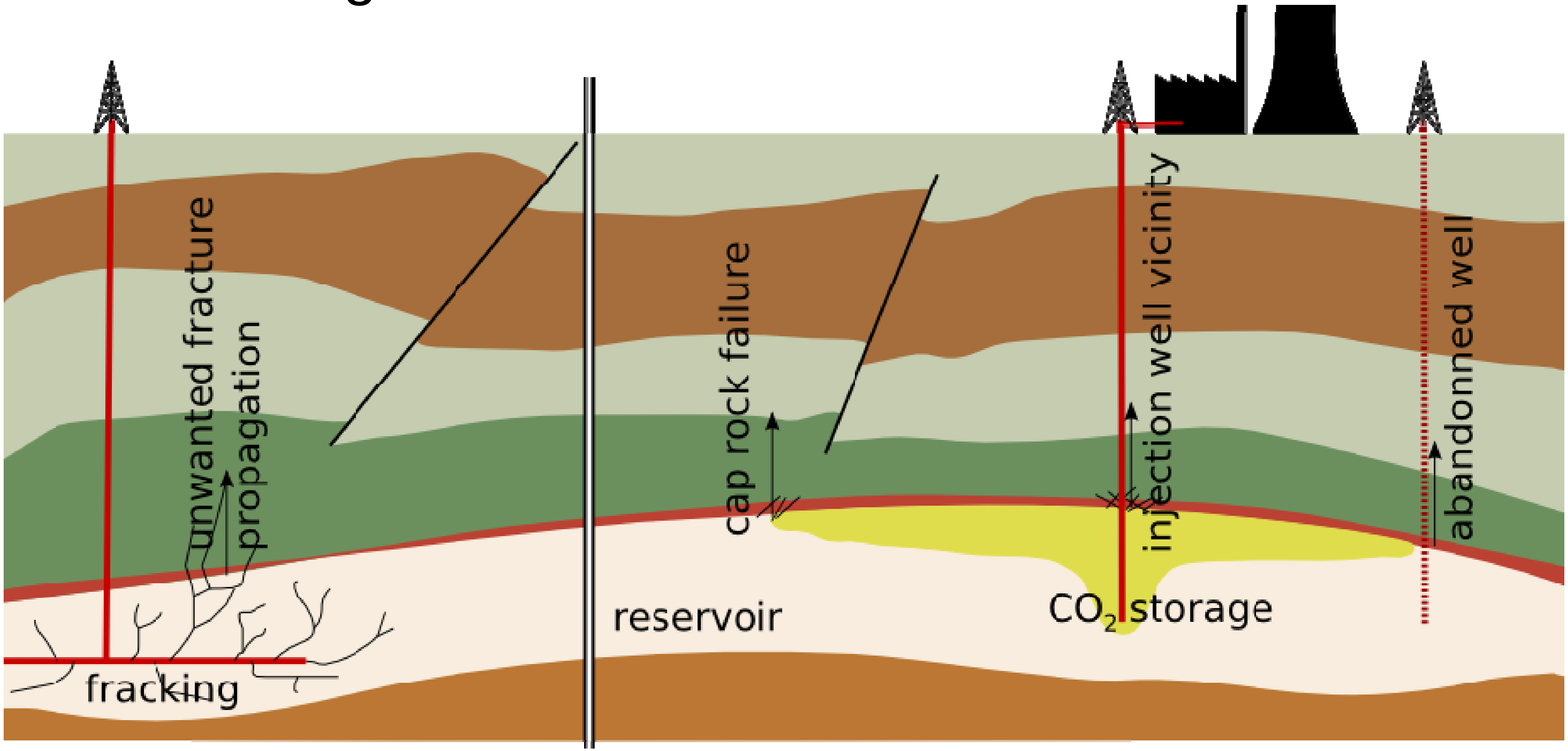
Motivation

Increased use of the subsurface injecting or extracting fluids.



Motivation

Increased use of the subsurface injecting or extracting fluids.

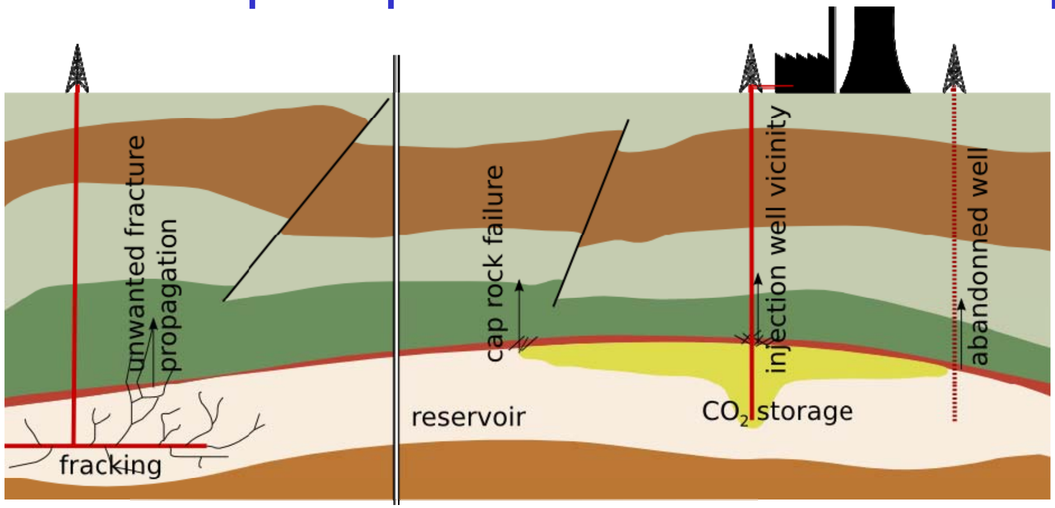
→ changing the chemistry of the pore water, which will re-equilibrate with the present minerals

→ need for reactive transport models

Exclusive and storage uses require separation.

→ sealing of leakage pathways is important

→ sealing is mineral precipitation = reactive transport



Outline

Model concept

Brief introduction to the model

Field scale simulations

Test the applicability of the model for large domains using the setting of a real field test site.

Challenges and solutions

Preliminary results

Summary and Outlook

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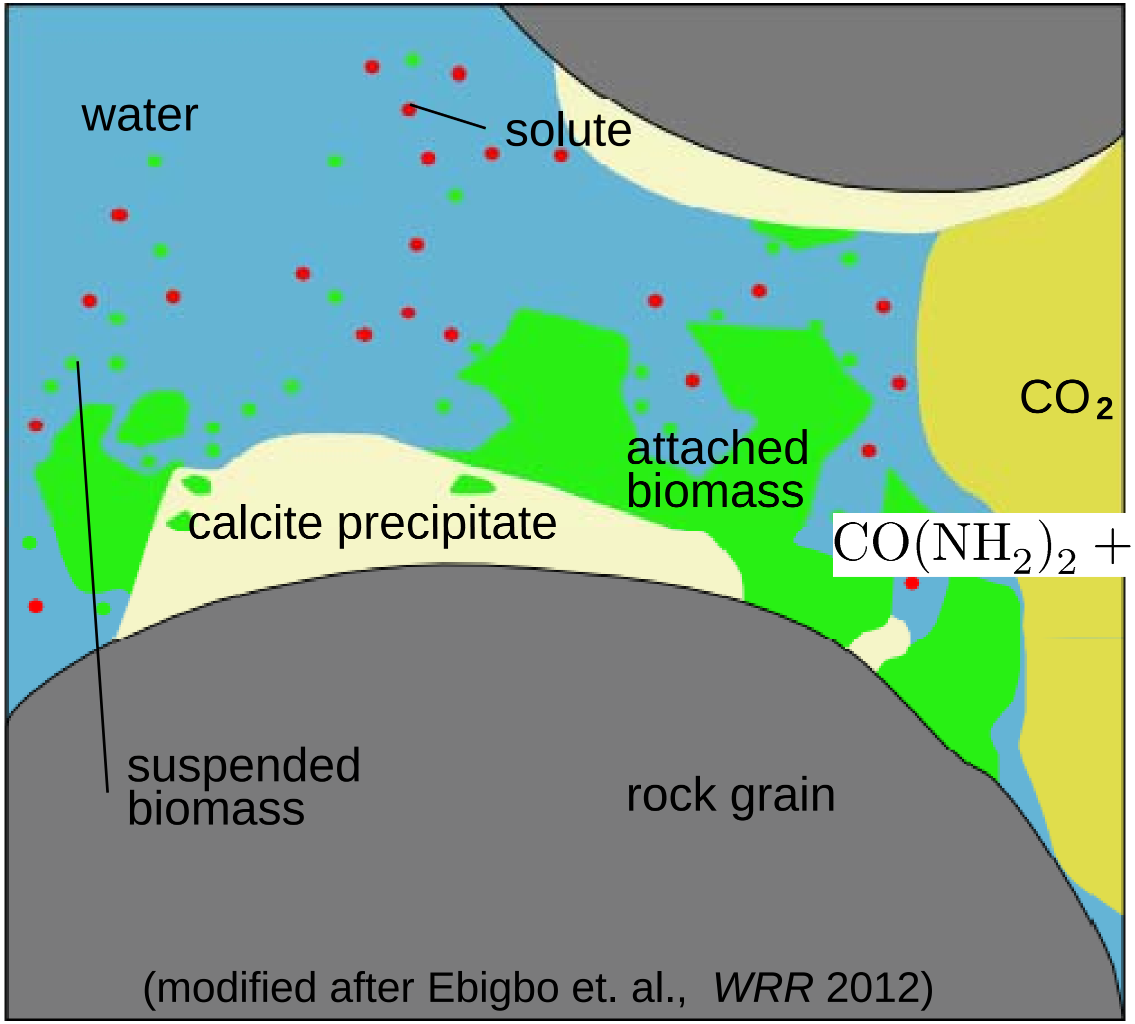
Model concept: Relevant processes



(modified after Ebigbo et. al., *WRR* 2012)

- Two-phase multi-component transport
- Biomass
  - growth / decay
  - attachment / detachment
- Urea hydrolysis

$$CO(NH_2)_2 + 2\,H_2O \xrightarrow{\text{urease}} 2\,NH_3 + H_2CO_3$$

- Precipitation / dissolution of calcite

$$Ca^{2+} + CO_3^{2-} \longleftrightarrow CaCO_3 \downarrow$$

- Clogging

$$\phi = \phi_0 - \phi_{\text{biofilm}} - \phi_{\text{calcite}}$$

$$K = K_0 \left(\frac{\phi - \phi_{\text{crit}}}{\phi_0 - \phi_{\text{crit}}}\right)^3$$

Model concept: important reactions

- Bacteria *Sporosarcina pasteurii* produce the enzyme urease.

- Urease catalyses the hydrolysis of urea, which produces ammonia and leads to a pH increase.

$$CO(NH_2)_2 + 2\,H_2O \xrightarrow{\text{urease}} 2\,NH_3 + H_2CO_3$$ ureolysis

$$H_2CO_3 \longleftrightarrow HCO_3^- + H^+$$ dissociation of carbonic acid

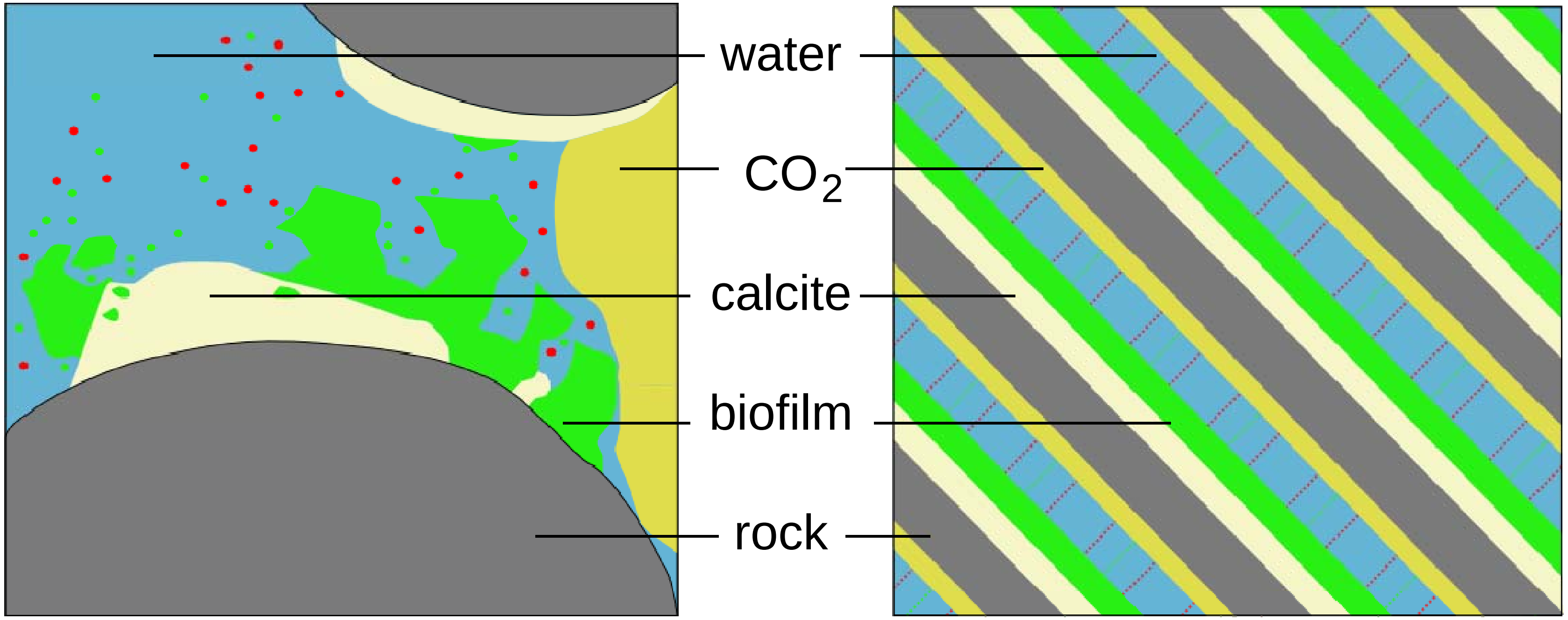
$$HCO_3^- \longleftrightarrow CO_3^{2-} + H^+$$ dissociation of bicarbonate ion

$$2\,NH_4^+ \longleftrightarrow 2\,NH_3 + 2\,H^+$$ dissociation of ammonia

$$Ca^{2+} + CO_3^{2-} \longleftrightarrow CaCO_3 \downarrow$$ calcite precipitation/dissolution

→ in the presence of calcium ions, the rise in pH due to ureolysis will drive the precipitation of calcite.

Model concept: Scale



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averaging

Pore scale → REV scale

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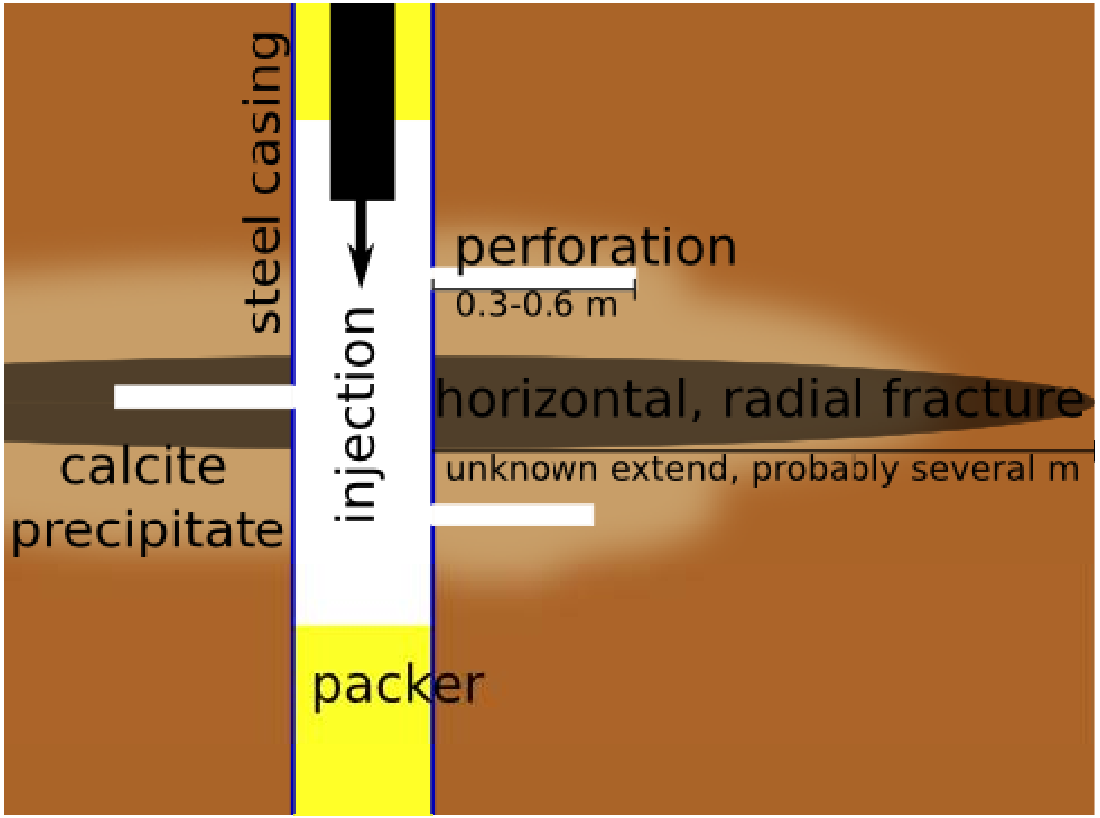
Field scale simulations, setup

- Test applicability of the model on a large scale
- Help design the actual experiment and interpret the results
- Uncertain geometry and injection strategy

→ different scenarios will be simulated

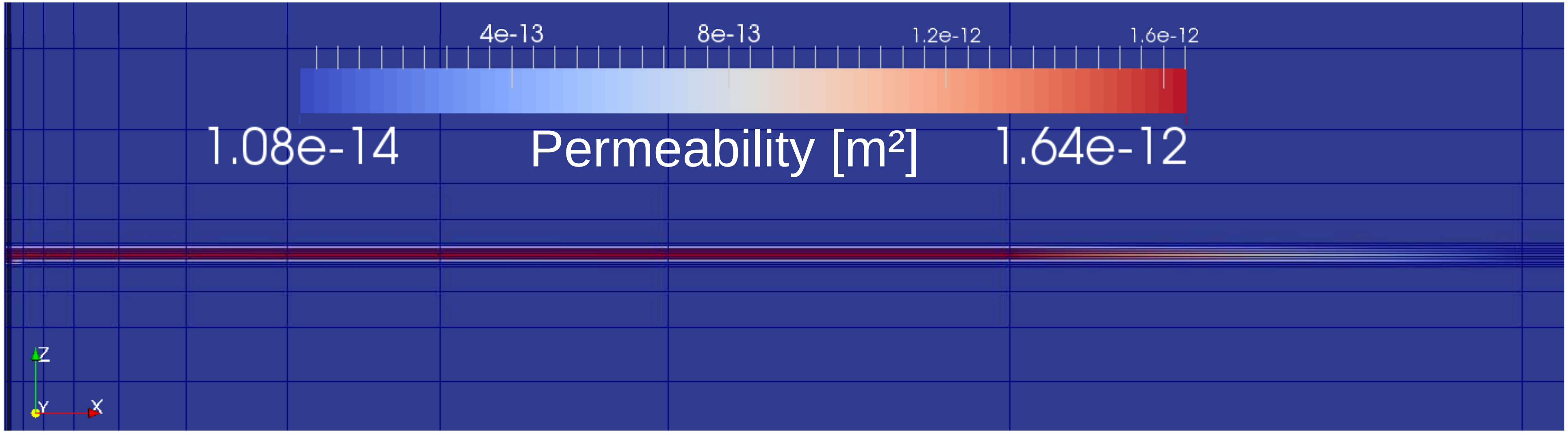


schematic view of the well and injection region

Simplifications of the setup

Simplifications:

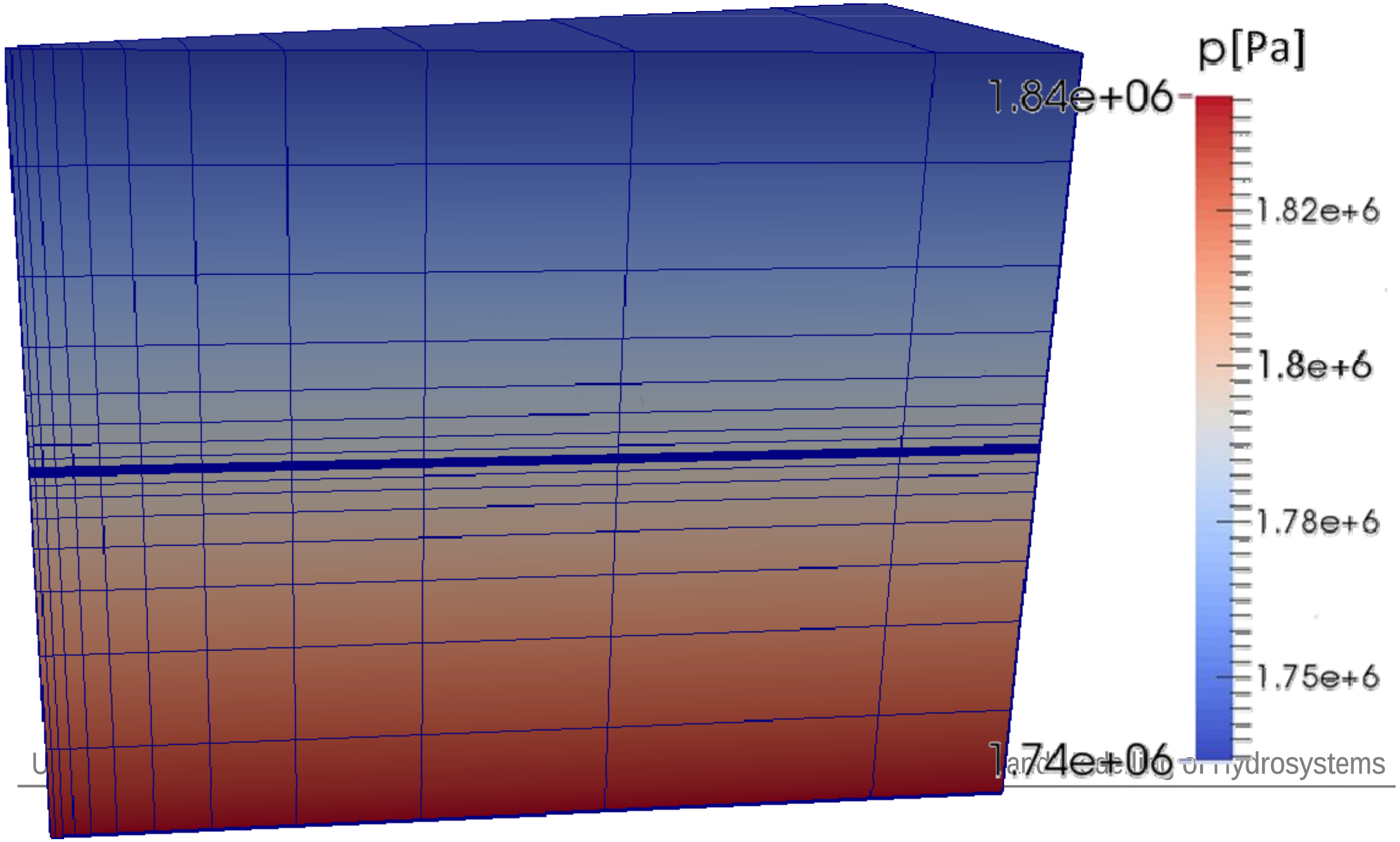
- No discrete fracture, but a horizontal high-permeability region



- radial, no perforation, but injection over the whole circumference

Field scale simulations

top, bottom, and sides: Neumann, q=0
outer radius: Dirichlet, values = initial
Inner radius: Neumann, q=0, except for injection into the high permeability region



Field scale simulations, challenge

CPU time in the order of days to weeks, caused by non-linear processes

- (biological and chemical, $CaCO_3$ precipitation in particular) and high number of unknowns.
- (10 components + 2 solid phases per node)

→ Parallel computing, decoupled transport and reactions
some speedup but CPU time remains in the range of days.

Field scale simulations, challenge

small volume, low pH, Ca^{2+} →

high CO_3^{2-} + Ca^{2+} → precipitation, but the rate is too high!	large volume, high pH → high CO_3^{2-}

A problem at larger scales is the increasing element size.

Dilution of small low pH, Ca^{2+}-rich volumes injected into large volumes of high pH brine leads to high CO_3^{2-} + relatively high Ca^{2+}

→ precipitation rates of up to 10^{12} mol/(m³s).

The molar density of pure calcite is only 27300 mol/m³!

→regularization of the precipitation rate,

→equilibrium instead of kinetic precipitation rate

Regularization

$$r_{\text{prec, kinetic}} = k_{\text{prec}} A_{\text{sw}} \left(\Omega - 1\right)^{n_{\text{prec}}}$$

$$r_{\text{prec, equilibrium}} = \text{molefraction}\left(m_{\text{prec}}\right) \frac{\rho_{\text{mol, brine}}}{\Delta t}$$

with:

$$m_{\text{prec}} = \frac{m_{\text{Ca}^{2+}} + m_{\text{CO}_3^{2-}} - \sqrt{\left(m_{\text{Ca}^{2+}} - m_{\text{CO}_3^{2-}}\right)^2 + 4 \frac{K_{\text{sp}}}{\gamma_{\text{Ca}^{2+}} \gamma_{\text{CO}_3^{2-}}}}}{2}$$

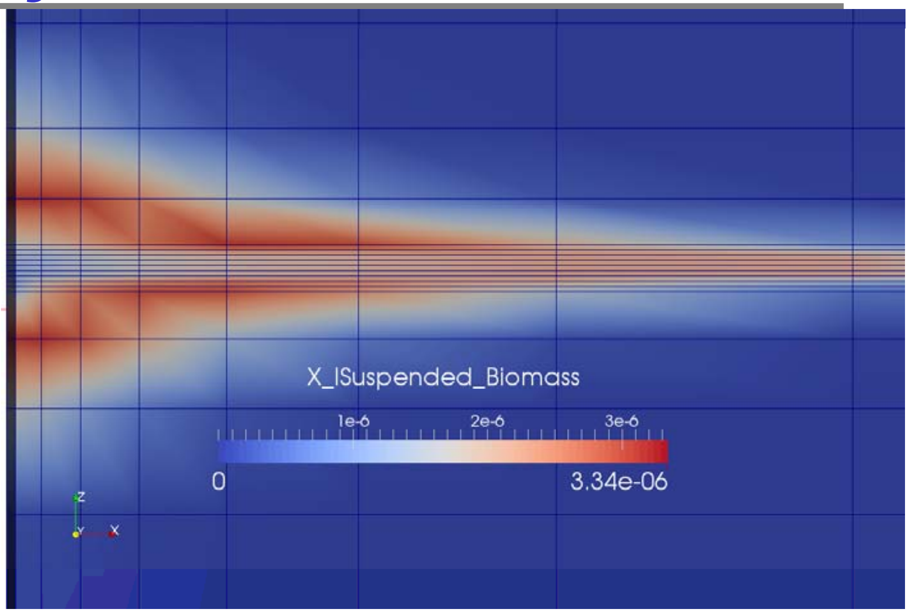
resulting from the assumption of equilibrium:

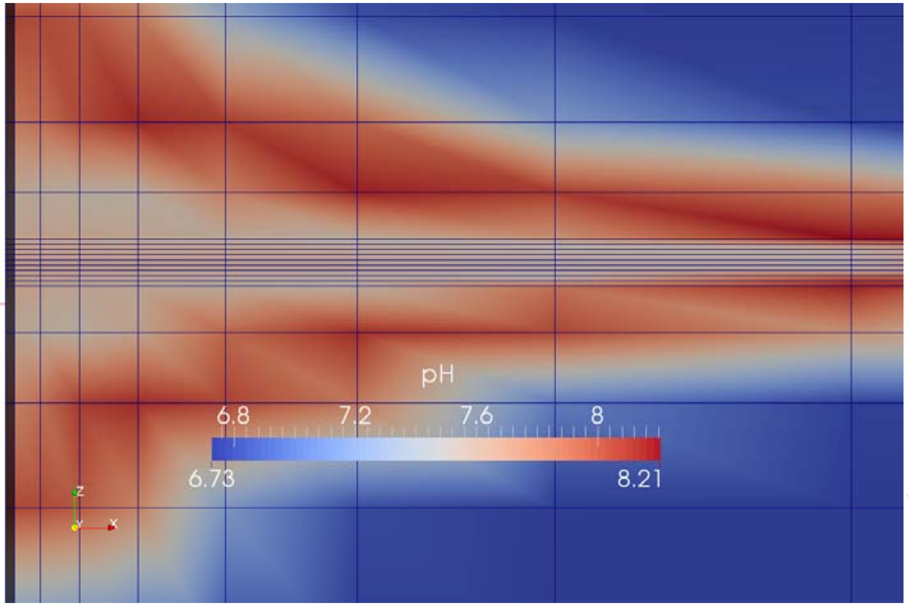
$$\left(m_{\text{Ca}^{2+}} - m_{\text{prec}}\right)\left(m_{\text{CO}_3^{2-}} - m_{\text{prec}}\right) = \frac{K_{\text{sp}}}{\gamma_{\text{Ca}^{2+}} \gamma_{\text{CO}_3^{2-}}}$$

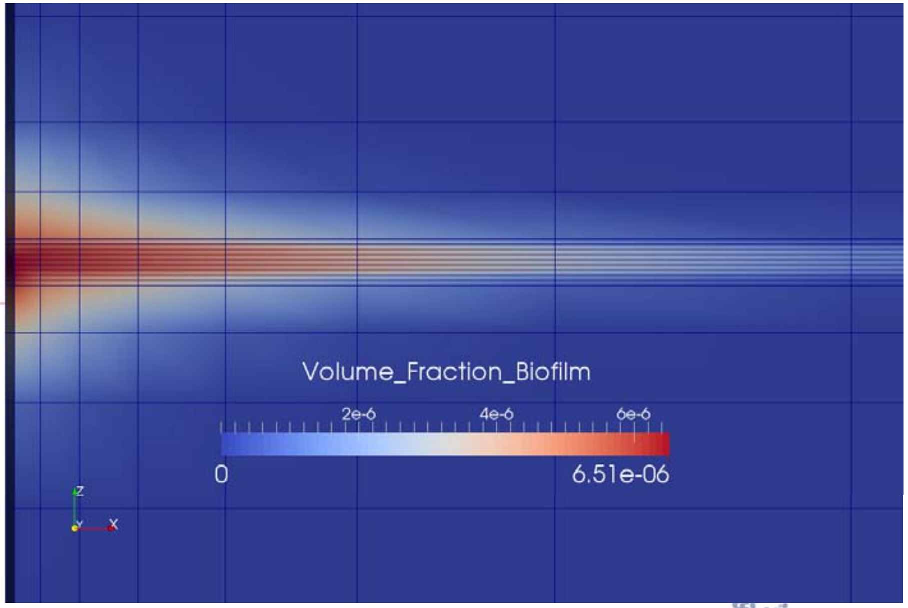
$$r_{\text{prec}} = \text{MIN}\left(r_{\text{prec, kinetic}}\ ,\ r_{\text{prec, equilibrium}}\right)$$

Preliminary results

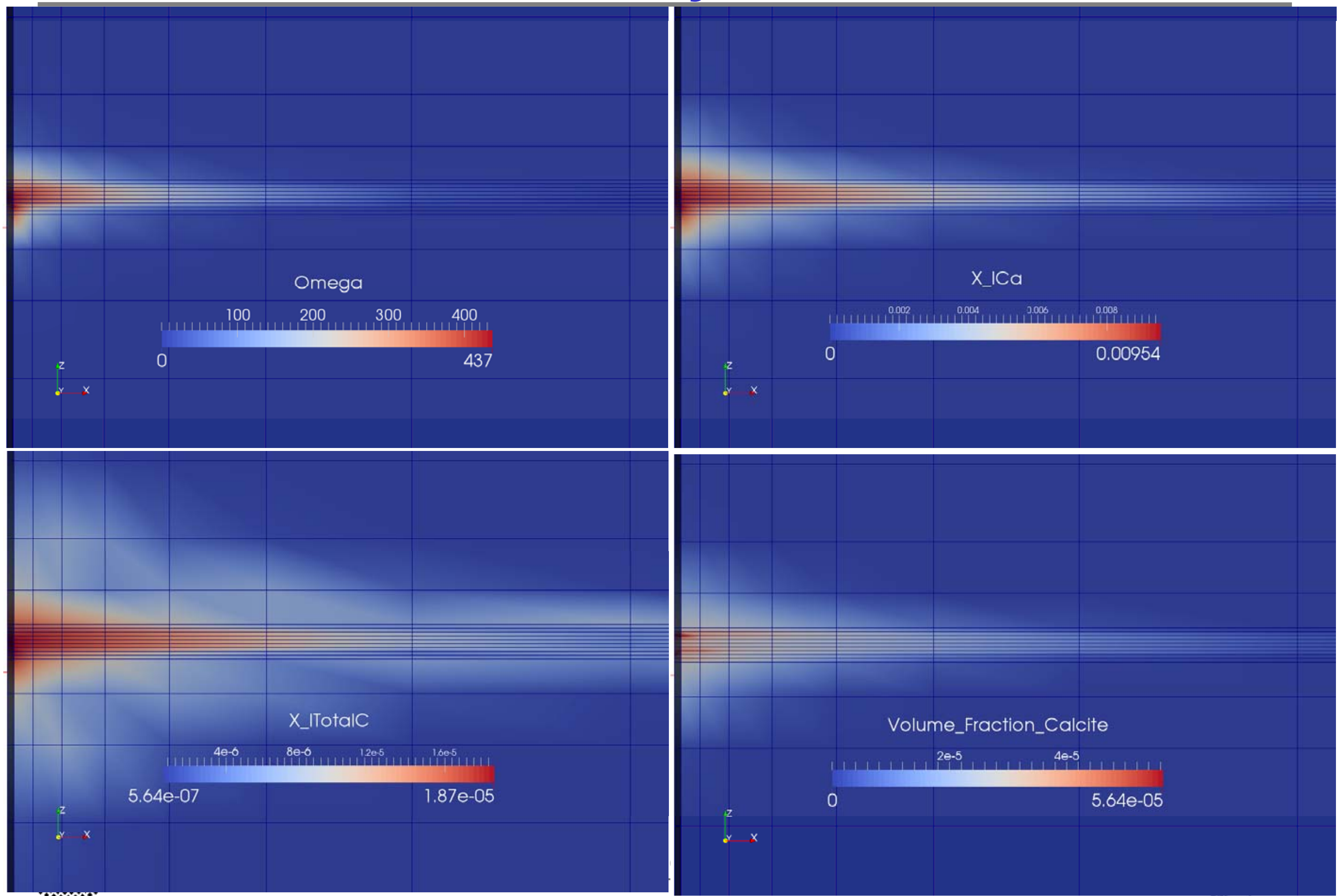
After first calcium-rich injection, t = 5 h.







Preliminary results



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- Transition from lab-scale to field-scale is not as simple as it seems in the first place.
- Discretization has a huge impact on modelled reaction rates (dilution effects) and thereby on the convergence behaviour and CPU time.
- Balance between CPU time and accuracy needs to be found by refining or coarsening the grid.

- In general, the model is applicable on larger scale, with constraints on grid size caused by both dilution effects and the number of nodes.

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Thank you for your attention!

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